```
=> s butylphthalide
L1          10 BUTYLPHTHALIDE

=> d 1-10

L1   ANSWER 1 OF 10  REGISTRY  COPYRIGHT 2009 ACS on STN
RN   879496-42-1  REGISTRY
ED   Entered STN:  06 Apr 2006
CN   2-Butenoic acid, 2-methyl-, 3-(1,3-dihydro-3-oxo-1-isobenzofuranyl)-1-
     methylpropyl ester, (2Z)-(-)-  (CA INDEX NAME)
OTHER NAMES:
CN   10-Angeloylbutylphthalide
FS   STEREOSEARCH
MF   C17 H20 O4
SR   CA
LC   STN Files:   CA, CAPLUS, TOXCENTER

Rotation (-).
Double bond geometry as shown.
Currently available stereo shown.
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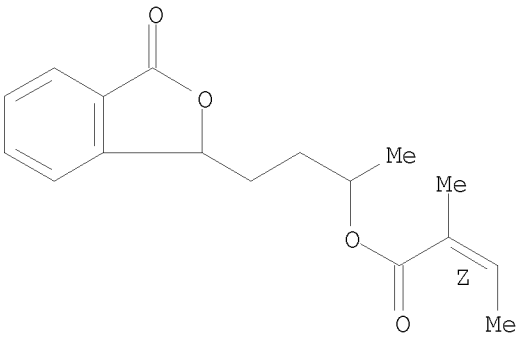


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               2 REFERENCES IN FILE CA (1907 TO DATE)
               2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1   ANSWER 2 OF 10  REGISTRY  COPYRIGHT 2009 ACS on STN
RN   199736-94-2  REGISTRY
ED   Entered STN:  14 Jan 1998
CN   1(3H)-Isobenzofuranone, 3-(2-methylpropyl)-  (CA INDEX NAME)
OTHER NAMES:
CN   3-Isobutylphthalide
MF   C12 H14 O2
SR   CA
LC   STN Files:   CA, CAPLUS
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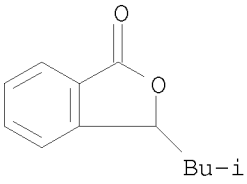
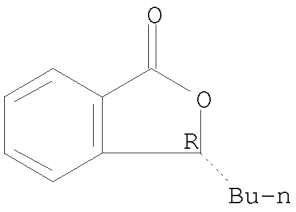


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 125412-70-6 REGISTRY
ED Entered STN: 16 Feb 1990
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1(3H)-Isobenzofuranone, 3-butyl-, (R)-
OTHER NAMES:
CN **(+)-3-Butylphthalide**
FS STEREOSEARCH
MF C12 H14 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).

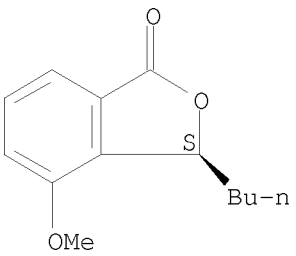


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

50 REFERENCES IN FILE CA (1907 TO DATE)
50 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 124831-75-0 REGISTRY
ED Entered STN: 19 Jan 1990
CN 1(3H)-Isobenzofuranone, 3-butyl-4-methoxy-, (S)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **(-)-4-Methoxy-3-butylphthalide**
FS STEREOSEARCH
MF C13 H16 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMINFORMRX

Absolute stereochemistry.

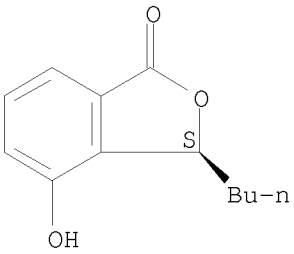


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 74459-24-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1(3H)-Isobenzofuranone, 3-butyl-4-hydroxy-, (3S)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1(3H)-Isobenzofuranone, 3-butyl-4-hydroxy-, (S)-
OTHER NAMES:
CN **(-)-4-Hydroxy-3-butylphthalide**
CN (3S)-3-Butyl-4-hydroxyphthalide
CN Chuangxinol
FS STEREOSEARCH
MF C12 H14 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

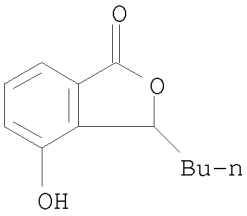
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)
10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

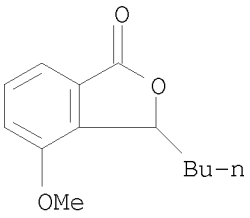
L1 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 74459-23-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1(3H)-Isobenzofuranone, 3-butyl-4-hydroxy- (CA INDEX NAME)
OTHER NAMES:
CN **4-Hydroxy-3-butylphthalide**
MF C12 H14 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, NAPRALERT, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES IN FILE CAPLUS (1907 TO DATE)

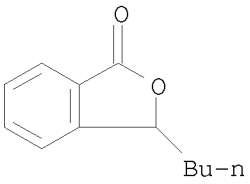
L1 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 74459-22-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1(3H)-Isobenzofuranone, 3-butyl-4-methoxy- (CA INDEX NAME)
OTHER NAMES:
CN **4-Methoxy-3-butylphthalide**
DR 150026-19-0
MF C13 H16 O3
LC STN Files: CA, CAPLUS, CASREACT, CHEMINFORMRX, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1907 TO DATE)
13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

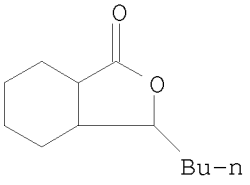
L1 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 6066-49-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phthalide, 3-butyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN **(±)-3-Butylphthalide**
CN 3-Butyl-1(3H)-isobenzofuranone
CN **3-Butylphthalide**
CN **3-n-Butylphthalide**
CN **Butylphthalide**
DR 93133-67-6
MF C12 H14 O2
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DDFU, DRUGU, EMBASE, IPA, MEDLINE, NAPRALERT, PROUSDDR, RTECS*, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

339 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
342 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 3553-34-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1(3H)-Isobenzofuranone, 3-butylhexahydro- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phthalide, 3-butylhexahydro- (8CI)
OTHER NAMES:
CN 3,n-Butylhexahydrophthalide
CN Cyclohexanecarboxylic acid, 2-(1-hydroxypentyl)-, γ-lactone
CN **Hexahydro-3-butylphthalide**
MF C12 H20 O2
LC STN Files: AGRICOLA, BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

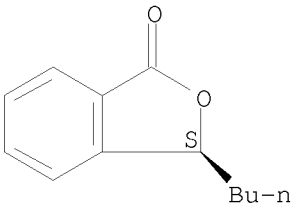


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

18 REFERENCES IN FILE CA (1907 TO DATE)
18 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2009 ACS on STN
RN 3413-15-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1(3H)-Isobenzofuranone, 3-butyl-, (S)-
CN Phthalide, 3-butyl-, (S)-(-)- (8CI)
OTHER NAMES:
CN **(-)-3-Butylphthalide**
CN **(3S)-Butylphthalide**
CN **(S)-3-Butylphthalide**
FS STEREOSEARCH
MF C12 H14 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX, EMBASE,
PROUSDDR, SYNTHLINE, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

72 REFERENCES IN FILE CA (1907 TO DATE)
72 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>
=> file caplus
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 38.33 | 38.55

FILE 'CAPLUS' ENTERED AT 11:49:26 ON 25 MAR 2009
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FILE LAST UPDATED: 24 Mar 2009 (20090324/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L2   404 L1

=> s l2 and pd<=2003
      23971199 PD<=2003
                  (PD<=20039999)
L3   256 L2 AND PD<=2003

=> s l3 and (l-butylphthalide or 125412-70-6 or 124831-75-0)
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L5 3 L4

   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L7 50 L6

1745557 L
310 BUTYLPHTHALIDE
8 BUTYLPHTHALIDES
314 BUTYLPHTHALIDE
(BUTYLPHTHALIDE OR BUTYLPHTHALIDES)
3 L-BUTYLPHTHALIDE
(L(W)BUTYLPHTHALIDE)
L8 37 L3 AND (L-BUTYLPHTHALIDE OR L7 OR L5)

=> focus
PROCESSING COMPLETED FOR L8
L9 37 FOCUS L8 1-

=> d ibib abs hitstr 1-37

L9 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:76923 CAPLUS
DOCUMENT NUMBER: 112:76923
ORIGINAL REFERENCE NO.: 112:13143a,13146a
TITLE: Preparation of 3-butylphthalide derivatives as prostaglandin F2α inhibitors
INVENTOR(S): Kubota, Kiyoshi; Ogawa, Yoshimitsu; Hosaka, Kunio; Chin, Masao
PATENT ASSIGNEE(S): Tsumura and Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 01050818	A	19890227	JP 1987-205216	19870820 <--
PRIORITY APPLN. INFO.:			JP 1987-205216	19870820
OTHER SOURCE(S):	MARPAT 112:76923			

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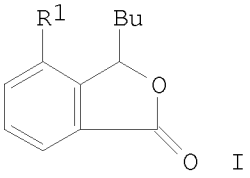


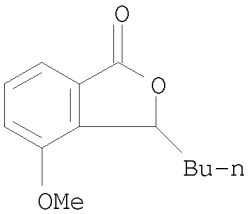
I

AB The title compds. (I; R1 = HO, MeO), which inhibit prostaglandin F2α and are useful for relaxing the smooth muscle of uterus and thus for treating abdominal pain associated with miscarriage, premature delivery, and disorders of uterus, are prepared Thus, treatment of 2-(3-methoxyphenyl)-4,4-dimethyl-2-oxazoline (preparation given) with BuLi followed by 2-valeraldehyde in THF at -45° gave 70% 2-[3-methoxy-2-(1-hydroxypentyl)phenyl]-4,4-dimethyl-2-oxazoline which was refluxed in 6N HCl to give 78% I (R1 = MeO) (II). Demethylation of the later with BBr3 in CH2Cl2 gave I (R1 = HO) (III). II, III and (-)-II in vitro at 5 + 10-8 g/mL inhibited prostaglandin F2α-induced contractility of rats' angular uterus by 35.3, 35.0 and 23.8%, resp. Tablets (200 mg) were formulated from II 5, corn starch 23.5, crystalline cellulose 158 CM-cellulose calcium salt 5, SO2 0.5, and Mg stearate 1 g.

IT **74459-22-6P**, 4-Methoxy-3-butylphthalide **74459-23-7P**, 4-Hydroxy-3-butylphthalide **74459-24-8P**, (-)-4-Hydroxy-3-butylphthalide **124831-75-0P**, (-)-4-Methoxy-3-butylphthalide
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as prostaglandin F2α inhibitor)

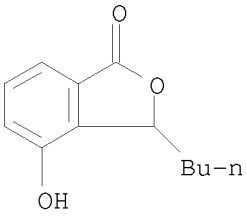
RN 74459-22-6 CAPLUS

CN 1(3H)-Isobenzofuranone, 3-butyl-4-methoxy- (CA INDEX NAME)



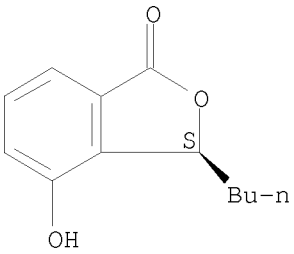
RN 74459-23-7 CAPLUS

CN 1(3H)-Isobenzofuranone, 3-butyl-4-hydroxy- (CA INDEX NAME)



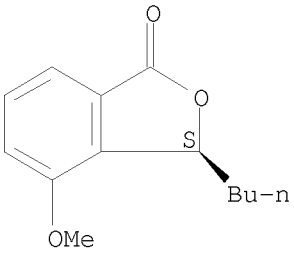
RN 74459-24-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-4-hydroxy-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 124831-75-0 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-4-methoxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

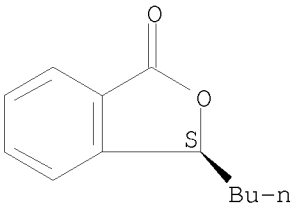


L9 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:104300 CAPLUS
DOCUMENT NUMBER: 134:125946
TITLE: Application of butylphthalide as antithrombotic and platelet aggregation inhibitor
INVENTOR(S): Feng, Yipu; Yang, Jinghua; Zhang, Yingxin
PATENT ASSIGNEE(S): Inst. of Medicinal Materials, Chinese Academy of Medical Sciences, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 16 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

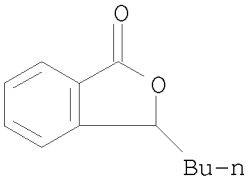
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1257706	A	20000628	CN 1998-125618	19981218 <--

CN 1086942 C 20020703
PRIORITY APPLN. INFO.: CN 1998-125618 19981218
AB Butylphthalide, preferably l-3-butylphthalide, is effective as antithrombotic and platelet aggregation inhibitor.
IT **3413-15-8 6066-49-5 125412-70-6**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(application of butylphthalide as antithrombotic and platelet aggregation inhibitor)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

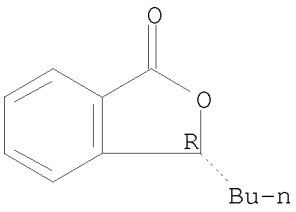


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:503839 CAPLUS
DOCUMENT NUMBER: 133:247088
TITLE: Protective effect of butylphthalide against mitochondrial injury during cerebral ischemia
AUTHOR(S): Xiong, Jie; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Science, Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**2000**), 35(6), 408-412
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Yaoxue Xuebao Bianjibu

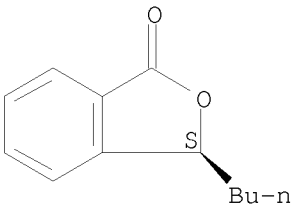
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The effects of butylphthalide (NBP) on the function and ultrastructure of neuronal mitochondria during cerebral ischemia were studied. Cerebral ischemia models of rat middle cerebral artery occlusion in vivo and primarily cultured neurons subjected to hypoxia/hypoglycemia in vitro were used. The mitochondria membrane fluidity (MMF) was determined by using fluorescent probes diphenylhexatriene (DPH). The mitochondria membrane potential (MMP) was measured with the fluorescence of loaded rhodamine-123 using flow cytometry. The total activity of mitochondria ATPase was measured. The morphol. changes of neuronal mitochondria were studied by using electron microscopy. The significantly enhanced value of n in the vehicle (MCAO) group showed that MMF was significantly decreased during the early stage of cerebral ischemia. MMP and total ATPase activity were decreased in rat fetal neurons subjected to 3 h-hypoxia/hypoglycemia. MMF after pretreatment with dl-NBP (5 mg kg-1 and 10 mg kg-1 i.p.) was close to that of the control level. MMP and ATPase activity were decreased by dl-, l-, and d-NBP. The severe swelling and marked vacuolation of mitochondria in morphol. were improved by NBP. The results suggest that the improving effects of NBP on mitochondrial injury and morphol. changes might contribute to its therapeutic action on exptl. stroke.

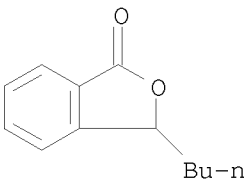
IT **3413-15-8, l-Butylphthalide 6066-49-5**
, Butylphthalide **125412-70-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(protective effect of butylphthalide against mitochondrial injury during cerebral ischemia)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

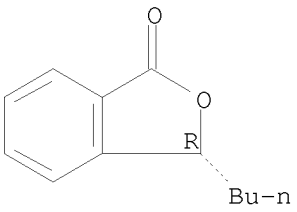


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:14692 CAPLUS
DOCUMENT NUMBER: 136:37499
TITLE: Process for preparing optically active 3-butylphenylphthalein as anticoagulant
INVENTOR(S): Yang, Jinhua; Zhang, Yingxin; Feng, Yipu
PATENT ASSIGNEE(S): Inst. of Medicinal Materials, Chinese Academy of Medical Sciences, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 16 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1283621	A	20010214	CN 1999-109673	19990705 <--
CN 1136208	C	20040128		

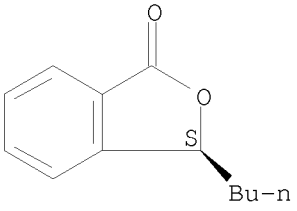
PRIORITY APPLN. INFO.: CN 1999-109673 19990705
OTHER SOURCE(S): CASREACT 136:37499

AB The resolution of chiral title compds., useful as anticoagulant (no data) in improving blockage of circulatory system in mammal, comprises ring-opening in solvent in the presence of base at 10-100°, regulating pH to 2.0-6.0 at (-20)-20°, extracting with extractant, solidifying with chiral amine, separating, regulating pH to 1.0-4.0, and cyclizing at 0-40°. The base is NaOH, KOH, Na2CO3, K2CO3, Na methoxide, or Na ethoxide. The solvent is methanol, ethanol, and/or water. The extractant is Et ether, Et acetate, chloroform, dichloromethane, benzene, toluene, petroleum ether, hexane, and/or pentane. The chiral amine is R1(R2)CHNH2 or R1(R2)CHNHR3 (R1 = H, C1-3 alkyl, hydroxymethyl, methoxymethyl, ethoxymethyl, acetoxymethyl, methoxycarbonyl, or ethoxycarbonyl; R2 = Ph, benzyl; and R3 = C1-3 alkyl, 2-hydroxyethyl).

IT **3413-15-8P 125412-70-6P**
RL: PNU (Preparation, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(process for preparing optically active 3-butylphenylphthalein as anticoagulant)

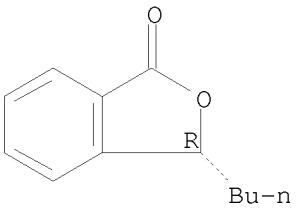
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

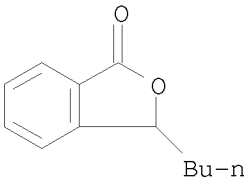


RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



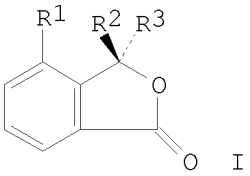
IT **6066-49-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparing optically active 3-butylphenylphthalein as anticoagulant)
RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



L9 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:98368 CAPLUS
DOCUMENT NUMBER: 112:98368
ORIGINAL REFERENCE NO.: 112:16727a,16730a
TITLE: Phthalides as prostaglandin F 2α inhibitors and their preparation
INVENTOR(S): Ogawa, Yoshimitsu; Chin, Masao; Hosaka, Kunio; Kubota, Kiyoshi
PATENT ASSIGNEE(S): Tsumura and Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01199958	A	19890811	JP 1987-182228	19870723 <--

PRIORITY APPLN. INFO.: JP 1987-182228 19870723
OTHER SOURCE(S): MARPAT 112:98368
GI



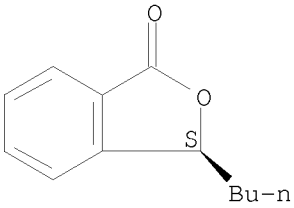
I

AB The title compds. I (R1 = H, MeO; when R2 is Bu, R3 is H, or when R2 is H, R3 = Bu; excluding the case where R1 = R2 = H and R3 = Bu), useful as prostaglandin F 2α inhibitors, were prepared A mixture of (-)-3-butyl-1-hydroxy-4-methoxy-2-oxaindan, AgNO3, and NaOH in MeOH-H2O was stirred at room temperature for 1 h to give (-)-4-methoxy-3-butylphthalide (II). II in vitro inhibited prostaglandin F 2α by 29.7%.

IT **3413-15-8P 124831-75-0P 125412-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as prostaglandin F 2α inhibitor)

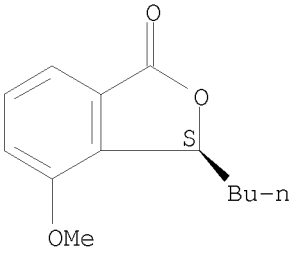
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



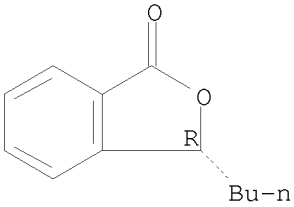
RN 124831-75-0 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-4-methoxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



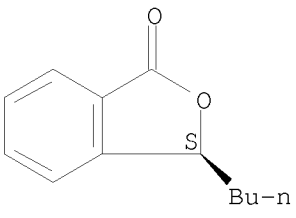
L9 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:651964 CAPLUS
DOCUMENT NUMBER: 140:174903
TITLE: Effects of chiral 3-n-butylphthalide on apoptosis induced by transient focal cerebral ischemia in rats
AUTHOR(S): Chang, Qing; Wang, Xiao-Liang
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Acta Pharmacologica Sinica (**2003**), 24(8), 796-804
CODEN: APSCG5; ISSN: 1671-4083
PUBLISHER: Science Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The purpose of this study was to investigate the effects of 3-n-butylphthalide (NBP) on apoptosis induced by transient focal cerebral ischemia in rats, compare the action potency of s-(-)-, r-(+)- and (±)-NBP, and clarify the enantiomer that played a main role. DNA fragmentation was detected by the terminal deoxynucleotidyl transferase-mediated biotinylated UTP nick end labeling (TUNEL) assay and gel electrophoresis. The expression of cytochrome c and caspase-3 protein was observed by Western blot anal. and immunohistochem. Middle cerebral artery was occluded for 2 h. Significant DNA fragmentation was detected at 24 h after reperfusion. This response was inhibited by s-(-)-NBP (5, 10 mg/kg i.p.). S-(-)-NBP 10 mg/kg almost completely inhibited DNA fragmentation, whereas r-(+)- NBP 10 mg/kg showed less effect. (±)-NBP (20 mg/kg) showed an inhibitory effect between that of s-(-)-NBP (10 mg/kg) and r-(+)-NBP (10 mg/kg). During the apoptotic process, cytochrome c was released into the cytosol and caspase-3 was activated. This effect was markedly inhibited by s-(-)-NBP, and the action potency of r-(+)- and (±)-NBP on the changes of cytochrome c and caspase-3 protein was similar to that on DNA fragmentation. NBP, especially its s-(-)-enantiomer, could potently reduce the release of cytochrome c, decrease the activation of caspase-3, and inhibit DNA fragmentation after transient focal cerebral ischemia. Our findings on the beneficial effects of NBP on cerebral ischemia-induced apoptosis might have important implications for the study and treatment of ischemic cerebrovascular diseases.

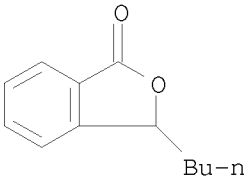
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, (.-+.)3-n-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: PAC (Pharmacological activity); BIOL (Biological study)
(effects of chiral 3-n-butylphthalide on apoptosis induced by transient focal cerebral ischemia in rats)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

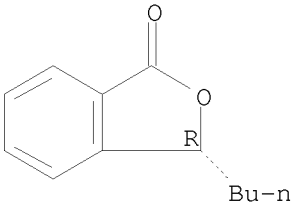


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

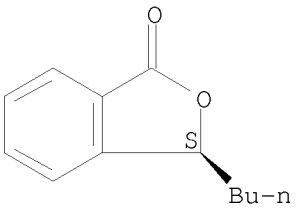
L9 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:646018 CAPLUS
DOCUMENT NUMBER: 139:403117
TITLE: Synthesis of covalently bonded cellulose derivative chiral stationary phases with a bifunctional reagent of 3-(triethoxysilyl)propyl isocyanate
AUTHOR(S): Chen, Xiaoming; Liu, Yueqi; Qin, Feng; Kong, Liang; Zou, Hanfa
CORPORATE SOURCE: Dalian Institute of Chemical Physics, National Chromatographic Research and Analysis Center, Chinese Academy of Sciences, Dalian, 116011, Peop. Rep. China
SOURCE: Journal of Chromatography, A (**2003**), 1010(2), 185-194
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A bifunctional reagent of 3-(triethoxysilyl)propyl isocyanate (TEPI) was initially adopted as a spacer reagent to prepare the bonded types of chiral stationary phases (CSPs) with cellulose derivs. The silica-based CSPs were chemical prepared with nonregioselective and regioselective approaches and their chiral resolving capabilities were evaluated in terms of HPLC resolution of test enantiomers. The chiral recognition capabilities of the nonregioselectively prepared CSPs were influenced by the amount of TEPI used. And also, the regioselectively prepared CSP generally showed a slightly higher resolution power than the nonregioselectively prepared CSP, while the nonregioselective procedures were highly advantageous to rapid preparation Chiral recognition of the prepared CSPs was affected by the properties of the used silica matrixes.

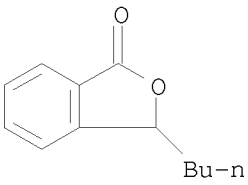
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, (±)-3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: ANT (Analyte); ANST (Analytical study)
(analyte; synthesis of covalently bonded cellulose derivative chiral stationary phases with a bifunctional reagent of (triethoxysilyl)propyl isocyanate for HPLC resolution of enantiomers)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

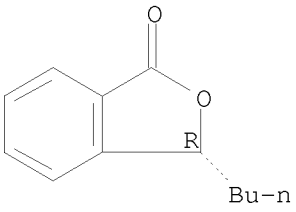


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

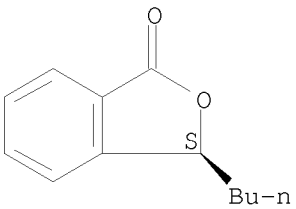
L9 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:309034 CAPLUS
DOCUMENT NUMBER: 138:241
TITLE: Effects of BP on ATPase and anti-oxidant enzymes activities and lipid peroxidation in transient focal cerebral ischemic rats
AUTHOR(S): Dong, Gaoxiang; Feng, Yipu
CORPORATE SOURCE: Department of Pharmacology, Institute of Materia Medica, CAMS and PUMC, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Yixue Kexueyuan Xuebao (**2002**), 24(1), 93-97
CODEN: CIHPDR; ISSN: 1000-503X
PUBLISHER: Zhongguo Yixue Kexueyuan
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The effects of 3-butylphthalide (BP) on ATPase, anti-oxidant enzymes activities, and lipid peroxidn. of mitochondria and cerebral cortex in

rats subjected to 24 h of reperfusion following 2 h of cerebral ischemia (tMCAO) were studied. Activities of SOD (superoxide dismutase), GSH-Px (glutathione Peroxidase), and CAT (catalase), and MDA level of mitochondria or cortex were measured by biochem. methods in tMCAO rats. The activities of mitochondrial Na+K+-ATPase, Ca2+- ATPase, and Mg2+-ATPase were decreased significantly in the vehicle group (ischemia-saline). Pre-treatment with BP (5, 10, and 20 mg kg-1, i.p.) 10 min before tMCAO remarkably enhanced the activities of Na+K+-ATPase and Ca2+-ATPase as compared with vehicle group. The activities of SOD and mitochondrial GSH-Px were decreased and MDA level increased in vehicle groups as compared with those in sham group (nonischemia-saline). BP (20 mg kg-1, i.p.) significantly enhanced total mitochondrial SOD activity, and also enhanced cerebral cortex total SOD activity (in 5, 10, and 20 mg kg-1 groups), but it had no obvious effect on CuZn-SOD activity. BP (20 mg kg1, i.p.) remarkably increased mitochondrial (but not in cerebral cortex) GSH-Px activity; BP (10 mg kg-1 and 20 mg kg-1) remarkably decreased mitochondrial MDA level as compared with that in vehicle group ($P < 0.05$). The action of racemic BP on the increase of the activities of ATPase and antioxidative enzymes was more beneficial than that of (-)-BP or (+)-BP. The results suggested that BP improved energy pump and subsided oxidative injury which may contribute to its anti-neuronal apoptotic effect.

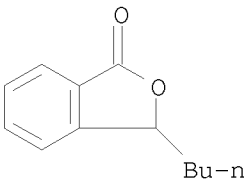
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, 3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of 3-butylphthalide on ATPase and anti-oxidant enzymes activities and lipid peroxidn. in transient focal cerebral ischemic rats)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

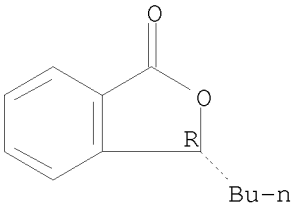


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



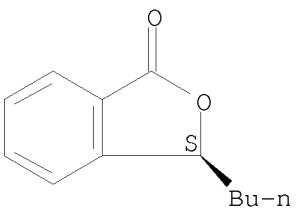
L9 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:534956 CAPLUS
DOCUMENT NUMBER: 136:288763
TITLE: Effects of 3-n-butylphthalide on thrombosis formation and platelet function in rats
AUTHOR(S): Xu, Haoliang; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**2001**), 36(5), 329-333
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Yaoxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The effects of dl-, l- and d-3-n-butylphthalide (NBP) on platelet aggregation and thrombus formation in rats were studied. Thrombus formation was measured by silk thread-induced thrombosis in arteriovenous shunt in rats. Rat platelet aggregation induced by ADP, arachidonic acid (AA), collagen, and thrombin was detected in vitro. The level of thromboxane B2 (TXB2) and concentration of cAMP in rabbit platelet in vitro were determined by RIA. The thrombus formation in rats was dose-dependently inhibited by dl- and l-NBP (5, 10, and 20 mg kg-1), but not by d-NBP. Platelet-rich plasma aggregation in vitro induced by ADP, collagen, and AA was inhibited by dl-, l-, and d-NBP (3-100 μM), but thrombin-induced platelet aggregation was not affected. The [cAMP]i was dose-dependently increased by dl-, l-, and d-NBP. The platelet TXA2 level was decreased only by high concentration of l-NBP. 5-HT release from platelet was significantly inhibited by l- NBP (1-100 μM), but not by dl-and d-NBP. The results showed that NBP was a potent antiplatelet drug, and its mechanism of antithrombotic and antiplatelet activities may be related to regulation of cAMP level and 5-HT release.

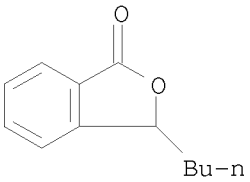
IT **3413-15-8**, (-)-3-Butylphthalide
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of 3-n-butylphthalide on thrombosis formation and platelet function in rats)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

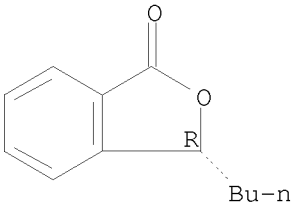


IT **6066-49-5**, 3-n-Butylphthalide **125412-70-6**,
(+)-3-Butylphthalide
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of 3-n-butylphthalide on thrombosis formation and platelet function in rats)
RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

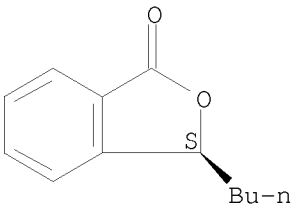


L9 ANSWER 10 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:737590 CAPLUS
DOCUMENT NUMBER: 134:50795
TITLE: Comparison of different di-tert-butyldimethyl-silylated cyclodextrins as chiral stationary phases in capillary gas chromatography
AUTHOR(S): Beck, Thomas; Liepe, Jens-Michael; Nandzik, Jan; Rohn, Sascha; Mosandl, Armin
CORPORATE SOURCE: Institut fur Lebensmittelchemie, Biozentrum J. W. Goethe-Universitat, Frankfurt/Main, D-60439, Germany
SOURCE: Journal of High Resolution Chromatography (**2000**), 23(10), 569-575
CODEN: JHRCE7; ISSN: 0935-6304
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Separation factors and thermodn. data for the separation of various chiral analytes
on different di-O-tert-butyldimethyl-silylated cyclodextrin derivs. are collected and described. Modifying the substitution pattern of the tert-butyldimethylsilyl group in position 2 and 3 or changing from β- to γ-cyclodextrin significantly affects the separation properties of the cyclodextrin derivs.
IT **3413-15-8**, (-)-3-Butyl phthalide **6066-49-5**,
(±)-3-Butyl phthalide **125412-70-6**, (+)-3-Butyl phthalide
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)

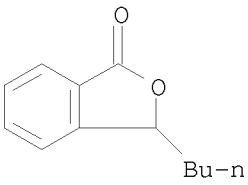
(analyte; comparison of different di-tert-butyldimethyl-silylated cyclodextrins as chiral stationary phases in capillary gas chromatog.)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

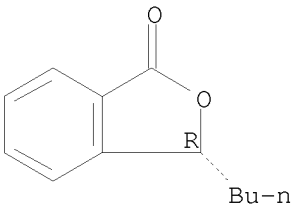


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

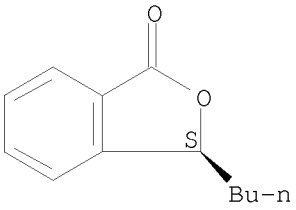
L9 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:676254 CAPLUS
DOCUMENT NUMBER: 134:231758
TITLE: Effects of DL-3-N-butylphthalide on arachidonic acid release and phospholipase A2 mRNA expression in cerebral cortex after middle cerebral artery occlusion in rats
AUTHOR(S): Chong, Zhaozhong; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**2000**), 35(8), 561-565
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Yaoxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of DL-3-n-butylphthalide (DL-NBP) on arachidonic acid (AA) release and phospholipase A2 (PLA2) mRNA in cerebral cortex of rats with focal cerebral ischemia was studied by HPLC for determination of AA and Northern blot for PLA2 mRNA expression. Focal cerebral ischemia was induced by inserting a monofilament nylon suture into the internal carotid artery and blocking the origin of the middle cerebral artery. AA release in the ischemic cerebral cortex after 6 h of cerebral ischemia was increased. AA concentration in the cerebral cortex was reduced by DL-NBP (10 or 20 mg kg-1, i.p.) and nimodipine (0.5 mg kg-1, i.p.). AA release in the brain after middle cerebral artery occlusion was decreased by D-NBP, but not by L-NBP. The expression of PLA2 mRNA in cerebral cortex induced by cerebral ischemia was inhibited by DL-NBP and D-NBP (10 or 20 mg kg-1, i.p.). The results showed that DL-NBP may inhibit AA release and PLA2 mRNA expression in the ischemic brain tissue in vivo.

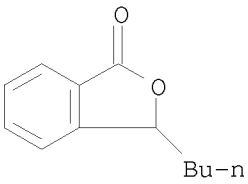
IT **3413-15-8 6066-49-5**, 3-N-Butylphthalide
125412-70-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(DL-3-N-butylphthalide on arachidonic acid release and phospholipase A2 mRNA expression in cerebral cortex after cerebral ischemia)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

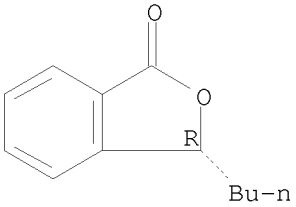


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

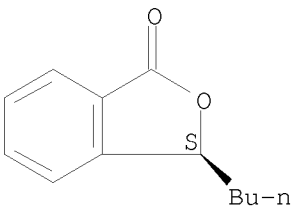
Absolute stereochemistry. Rotation (+).



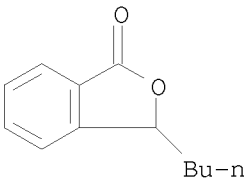
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:303339 CAPLUS
DOCUMENT NUMBER: 133:84030
TITLE: Inhibitory effects of chiral 3-n-butylphthalide on inflammation following focal ischemic brain injury in rats
AUTHOR(S): Xu, Hao-Liang; Feng, Yi-Pu
CORPORATE SOURCE: Institute of Materia Medica, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing, 100050, Peop. Rep. China
SOURCE: Acta Pharmacologica Sinica (**2000**), 21(5), 433-438
CODEN: APSCG5
PUBLISHER: Science Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB AIM: To evaluate the degree of neutrophil infiltration into ischemic tissue after transient focal cerebral ischemia, and to examine the effects of chiral 3-n-butylphthalide (NBP) on this inflammatory process. METHODS: After a 24-h reperfusion following transient cerebral ischemia, two different techniques, histol. anal. and modified myeloperoxidase (MPO)-quantification method, were utilized to identify the infiltration of neutrophils into cerebral tissue following ischemia. The expression of intercellular adhesion mol.-1 (ICAM-1) and tumor necrosis factor-α(TNF-α) in the ischemic zone were observed by immunohistochem., Western blot, and in situ hybridization techniques. RESULTS: In cerebral cortex area perfused by middle cerebral artery (MCA), MPO activity was greatly increased after 24 h of reperfusion in the vehicle group, and it correlated well with the infiltration of neutrophils. Administration of dl-, d-, and l-NBP (20 mg·kg-1) partially inhibited both the increase in MPO activity and the appearance of neutrophils in ischemia-reperfusion sites. Upregulation of ICAM-1 was also observed on the microvessel endothelium in the ischemic territory. In addition, chiral NBP markedly blunted ICAM-1 expression, and decreased the number of TNF-α blue purple-pos. neurons induced by ischemia-reperfusion injury. CONCLUSION: The results indicate that the increase in neutrophils infiltration into the infarct site implicated postischemic brain injury, and NBP was effective in protecting the ischemic sites following ischemic insult.
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, 3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chiral 3-n-butylphthalide inhibition of inflammation after focal ischemic brain injury)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

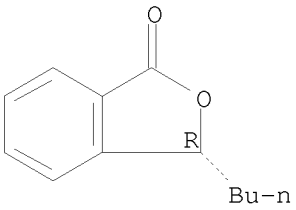


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

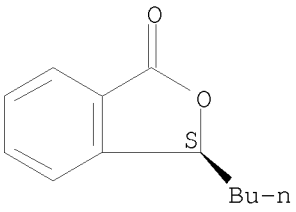


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

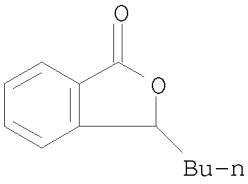
L9 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:90975 CAPLUS
DOCUMENT NUMBER: 133:38056
TITLE: Effects of 3-n-butylphthalide on increase of intracellular calcium in neurons subjected to hypoxia and hypoglycemia and its mechanisms
AUTHOR(S): Xiong, Jie; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**1999**), 34(12), 893-897
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Yaoxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The decreasing effects and the mechanisms of d-, l-, and dl-butylphthalide (NBP) on intracellular calcium ([Ca2+]i) in neurons subjected to hypoxia and hypoglycemia were studied by using Fura-2/AM as fluorescence indicator for studying the actions of NBP on [Ca2+]i, and thapsigargin, glutamine, KCl or calcium ionophore A23187 as tool drugs for analyzing the mechanisms of the action of chiral NBP. The increase of intracellular calcium caused by hypoxia and hypoglycemia was significantly inhibited by d-, l- and dl-NBP. The increase of [Ca2+]i induced by the tool drugs except thapsigargin was not affected by chiral NBP, but that induced by glutamate was inhibited by d-NBP. The results showed that the actions of d-, l- and dl-NBP might be mediated mainly by its decreasing effect on the release of calcium from intracellular calcium pool.
IT **3413-15-8 6066-49-5**, 3-n-Butylphthalide
125412-70-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effects of 3-n-butylphthalide on increase of intracellular calcium in

neurons subjected to hypoxia and hypoglycemia and its mechanisms)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

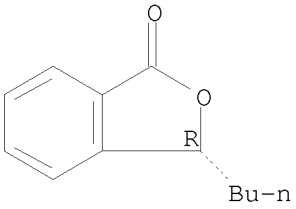


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



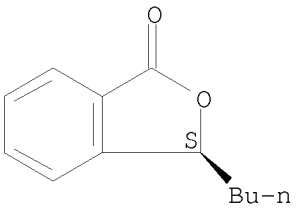
L9 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:18352 CAPLUS
DOCUMENT NUMBER: 132:274050
TITLE: Effects of 3-n-butylphthalide on neutrophil-endothelial cell adhesion and endothelial cell injury induced by anoxia/reoxygenation, interleukin-1 and tumor necrosis factor-α
AUTHOR(S): Xu, Hao-Liang; Feng, Yi-Pu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Yaolixue Yu Dulixue Zazhi (**1999**), 13(4), 281-284
CODEN: ZYYZEW; ISSN: 1000-3002
PUBLISHER: Zhongguo Yaolixue Yu Dulixue Zazhi Biarjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The effects of dl-, d-, 1-3-n-butylphthalide (NBP) on interleukin-1 (IL-1), tumor necrosis factor-α (TNF-a), anoxia/reoxygenation

induced neutrophil adhesion to endothelial cells (ECs) and EC cytotoxicity were studied. ECs from bovine aortic artery cords were isolated and cultured in vitro, and then were subjected to anoxia in an anaerobic chamber for 3 h followed by 3 h of reoxygenation, or stimulated by IL-1 (200 kU · L-1) and TNF-α (200 kU · L-1), resp. for 24 h. The percentage of neutrophils that adhered to the EC monolayers was measured by myeloperoxidase-quantified method. Cytotoxicity of ECs was determined by the method of MTT. Along with incubation under anoxia/reoxygenation, a dramatical increase in adherence of neutrophils to ECs was observed Similar results were observed with respect to neutrophil-EC adhesion promoted by IL-1, TNF-α. Hyper-adherence induced by IL-1, anoxia/reoxygenation was significantly diminished following pretreatment with d-NBP given 1 h before stimuli, however, the increased adhesion induced by TNF-a was unchanged. Cytotoxicity studies demonstrated that anoxia/reoxygenation, IL-1 and TNF-α elicited the marked EC injury, and incubation of ECs with dl-, l-, d-NBP prior to these stimuli could partially blunted this injury. These findings indicate that d-NBP attenuates the neutrophil-EC adhesion elicited by anoxia/reoxygenation, IL-1. Furthermore, dl, l, d-NBP blunt the EC injury induced by anoxia/reoxygenation, IL-1 and TNF-α.

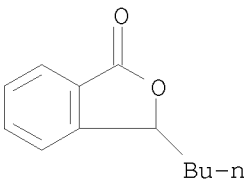
IT **3413-15-8 6066-49-5**, 3-n-Butylphthalide
125412-70-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of 3-n-butylphthalide on neutrophil-endothelial cell adhesion and endothelial cell injury induced by anoxia/reoxygenation, interleukin-1 and tumor necrosis factor-α)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

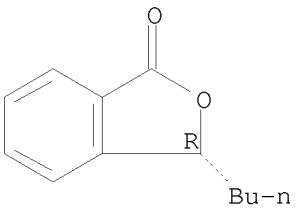


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

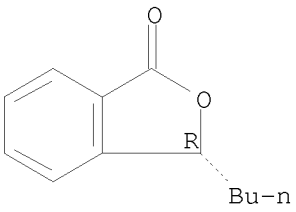


L9 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:758599 CAPLUS
DOCUMENT NUMBER: 132:274163
TITLE: Effects of 3-n-butylphthalide on release of glutamate and 5-HT from cultured neurons subjected to hypoglycemia/hypoxia
AUTHOR(S): Chong, Zhaozhong; Feng, Yipu
CORPORATE SOURCE: Institute of Material Medica, Chinese Academy of Medical Sciences, Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Yaoxue Zazhi (Beijing) (**1999**), 34(9), 589-591
CODEN: ZYZAEU; ISSN: 1001-2494
PUBLISHER: Zhongguo Yaoxuehui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The effects of dl-3-n-butylphthalide (dl-NBP), d-NBP and l-NBP on the release of glutamate and 5-hydroxytryptamine (5-HT) from cultured perinatal cortical neurons were studied. The cortical neurons were cultured with medium containing low glucose and bubbled with N2, glutamate and 5-HT were determined fluorometrically. The results showed that dl-NBP (1 and 10 μmol L-1) and l-NBP (10 μmol L-1) reduced the glutamate release and the release of 5-HT from cultured cortical neurons induced by hypoglycemia/hypoxia for 10 h. D-NBP had no significant effect. dl-NBP and l-NBP also decreased the glutamate release induced by arachidonic acid (100 μmol L-1). The inhibitory effects of NBP on the release of glutamate and 5-HT might be one of its action mechanisms in the treatment of cerebral ischemia.

IT **125412-70-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effects of 3-n-butylphthalide on release of glutamate and 5-HT from cultured neurons subjected to hypoglycemia/hypoxia)
RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

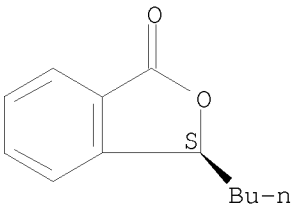


IT **3413-15-8 6066-49-5**, 3-n-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

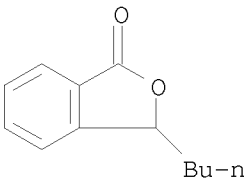
(effects of 3-n-butylphthalide on release of glutamate and 5-HT from cultured neurons subjected to hypoglycemia/hypoxia)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



L9 ANSWER 16 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:581193 CAPLUS
DOCUMENT NUMBER: 132:131676
TITLE: Effect of dl-3-n-butylphthalide on activity of choline acetyltransferase in ischemic brain and cultured neurons subjected to hypoglycemia/hypoxia
AUTHOR(S): Chong, Zhaozhong; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Yaoxue Zazhi (Beijing) (**1999**), 34(8), 519-522
CODEN: ZYZAEU; ISSN: 1001-2494
PUBLISHER: Zhongguo Yaoxuehui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

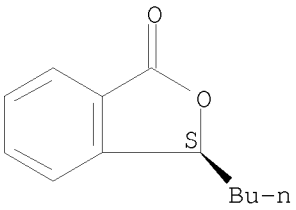
AB The effects of dl-3-n-butylphthalide (dl-NBP), d-NBP and l-NBP on the activity of choline acetyltransferase (ChAT) in ischemic brain and cultured neurons subjected to hypoglycemia/hypoxia were studied by examining the activity of ChAT with spectrophotometry. The activity of ChAT was decreased by 61.3% and 58.4%, resp., in cerebral cortex and striatum after 6 h of blockade of the origin of middle cerebral artery. dl-NBP, d-NBP and l-NBP increased ChAT activity in ischemic brain and improved ChAT activity in cultured perinatal rat cortical neurons subjected to hypoglycemia/hypoxia or NMDA treatment. The results showed that the effect of dl-NBP on learning and memory function impaired by focal cerebral ischemia may be related to its protective effect on the activity of choline acetyltransferase.

IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, 3-n-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

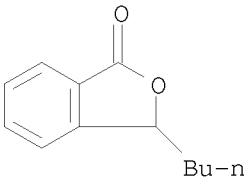
(Uses)
(effect of butylphthalide on choline acetyltransferase activity in ischemic brain and neuronal injury)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

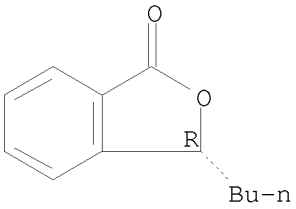


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



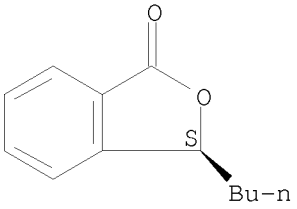
L9 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:405281 CAPLUS
DOCUMENT NUMBER: 131:317711
TITLE: Anticonvulsant effects of 3-n-butylphthalide and its optical isomers
AUTHOR(S): Dong, Gaoxiang; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Yaolixue Tongbao (**1999**), 15(1), 88-89
CODEN: ZYTOE8; ISSN: 1001-1978
PUBLISHER: Anhui Yike Daxue Linchuan Yaoli Yanjiuso
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The anticonvulsant effects of 3-n-butylphthalide (NBP) and its d- and l-isomers were studied in mice with electroshock- and metrazole-induced

convulsions. The anticonvulsant activities against maximal electroshock seizure were in the order dl-NBP > d-NBP > l-NBP, with ED50 values of 73.1 mg/kg, 83.4 mg/kg and 104.8 mg/kg, resp.; the effects were dose dependent. None of the compds. was as active as Na phenobarbital. NBP and its isomers, at doses of ≤250 mg/kg, were inactive against metrazole-induced convulsions.

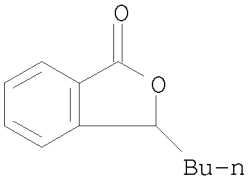
IT **3413-15-8**, l-3-n-Butylphthalide **6066-49-5**, 3-n-Butylphthalide **125412-70-6**, d-3-n-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(anticonvulsant effects of butylphthalide and its optical isomers)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

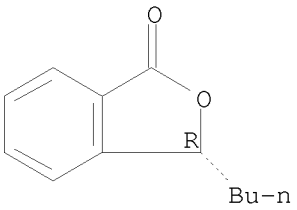


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

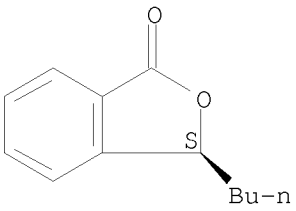
Absolute stereochemistry. Rotation (+).



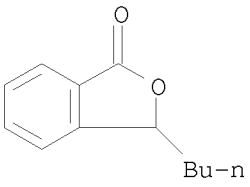
L9 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:356180 CAPLUS
DOCUMENT NUMBER: 131:209011
TITLE: Effects of butylphthalide on activities of complexes of mitochondrial respiratory chain
AUTHOR(S): Xiong, Jie; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Media, Chinese Academy of Medical Sciences, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**1999**), 34(4), 241-245

CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Yaoxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The effects of dl-3-n-butylphthalide (dl-NBP) on the function of mitochondrial respiratory chain were studied by determination of the activities of the four complexes of the respiratory chain. The decreased activity of complex IV after 1 h-ischemia was returned to normal level by treatment of NBP (5 mg.kg-1 i.p. or 10 mg.kg-1 10 min before ischemia). The activity of complex I was significantly increased at 3 h, and that of complex II was decreased at 6 h during the reperfusion period after ischemia; the altered activities may returned to normal by treatment of NBP. The same increasing effect of NBP (d-, l- or dl-) on the activity of complex IV was found in cultured neurons subjected to 6 h-hypoxia/hypoglycemia, and d-NBP was more effective. The results indicated that NBP can act directly on complex IV to increase its activity, and its action may play an important role in increasing brain energy supply during cerebral ischemia.
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, 3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of butylphthalide on activities of complexes of mitochondrial respiratory chain)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

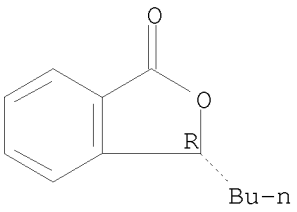


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



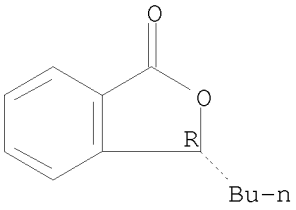
L9 ANSWER 19 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:280032 CAPLUS
DOCUMENT NUMBER: 131:139336
TITLE: Effects of 3-n-butylphthalide on pial microcirculation dysfunction in rats with focal cerebral ischemia
AUTHOR(S): Xu, Haoliang; Feng, Yipu
CORPORATE SOURCE: Institute of Material Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**1999**), 34(3), 172-175
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Yaoxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The effects of dl-, l-, and d-3-n-butylphthalide (NBP) on pial arteriole diameter (AD) and blood flow velocity (BFV) in rats with focal cerebral ischemia were studied. The effects of dl-NBP, l-NBP and d-NBP on AD and BFV were investigated in the left middle cerebral artery occluded (L-MCAO) rats anesthetized with urethane by using the method of acute cranial window technique under in vitro videomicroscope. dl-NBP, d-NBP and l-NBP (25 mg kg-1 i.p.) and nimodipine were administered 20 min after MCAO or 1 h before MCAO. In the vehicle control group, MCAO decreased BFV and AD by 18.3% and 52% resp., compared with the pre-ischemia baseline values. In the pretreatment groups, no change in pial AD was found after dl-NBP, l-NBP, d-NBP administration in normal animals, and a rapid and marked decrease in BFV and Ad of the selected pail artery was observed within 5 min after MCAO. The decreased level of AD and BFV recovered quickly after MCAO in the dl-, l-NBP and nimodipine groups, while the dysfunction of microcirculation was exacerbated by d-NBP. In the post-treatment groups, dl-NBP (12.5, 25 mg kg-1 i.p.) induced dilation of the pial arterioles and the increase in BFV was in dose-dependent manner. The pial arteriolar response to MCAO was no affected by d-NBP and nimodipine. These data suggested that the improving effects of dl-NBP and l-NBP on microcirculation dysfunction during ischemia might play an important role in their protective effects against focal cerebral ischemia injury. L-NBP and d-NBP showed counteractive effect on pial AD and BFV in MCAO rats indicating that NBP has stereoselective characters on its protective action against cerebral ischemia injury.

IT **125412-70-6**, d-3-n-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(effects of 3-n-butylphthalide on pial microcirculation dysfunction in rats with focal cerebral ischemia)

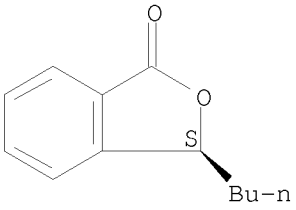
RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

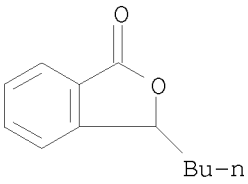


IT **3413-15-8**, l-3-n-Butylphthalide **6066-49-5**,
3-n-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of 3-n-butylphthalide on pial microcirculation dysfunction in rats with focal cerebral ischemia)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



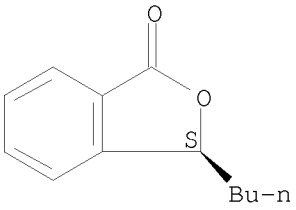
L9 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:88971 CAPLUS
DOCUMENT NUMBER: 131:521
TITLE: Effects of butylphthalide on extracellular 6-keto-PGF1α, TXB2 and 6-keto-PGF1α/TXB2 ratio in cultured rat cortical neurons
AUTHOR(S): Yan, Chaohua; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**1998**), 33(12), 881-885
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The effects of 3-n-butylphthalide (NBP) on the levels of 6-keto-PGF1α, TXB2 and 6-keto-PGF1α/TXB2 ratio were studied

with RIA methods. D-NBP and l-NBP (0.1-100 μmol L-1) concentration-dependently increased 6-keto-PGF1α release, decreased TXB2 release from neuronal cells, and significantly enhanced extracellular 6-keto-PGF1α/TXB2 ratio in primary cultured rat cortical neurons exposed to hypoglycemic and hypoxic media for 5 h or hypoxic-hypoglycemic media for 5 h following normal media for 3 h. Aspirin (0.1-100 μmol L-1) was also shown to inhibit TXB2 release from cortical neurons in a dose-dependent manner. However aspirin only increased 6-keto-PGF1α/TXB2 ratio at low dose because aspirin inhibited both 6-keto-PGF1α and TXB2 release simultaneously at large dose (10-100 μmol L- 1). This suggested that the increase of 6-keto-PGF1α/TXB2 ratio by l-NBP, d-NBP and dl-NBP might be due to NBP enhancing focal cerebral blood flow and improving ischemic brain damage.

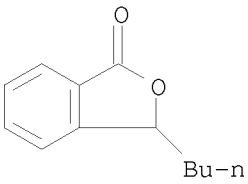
IT **3413-15-8 6066-49-5**, Butylphthalide **125412-70-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(butylphthalide effects on extracellular 6-keto-PGF1α, TXB2 and 6-keto-PGF1α/TXB2 ratio in cultured rat cortical neurons in relation to enhanced cerebral blood flow and improving ischemic brain damage)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

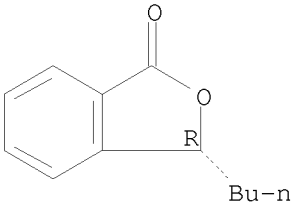


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



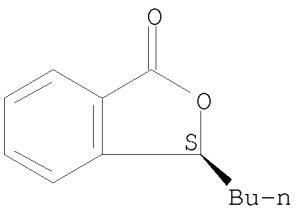
L9 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:808407 CAPLUS
DOCUMENT NUMBER: 130:261906
TITLE: Protective effects of d-, l-, and dl-3-n-butylphthalide on neuronal damage induced by hypoxia/hypoglycemia in cultured rat cortical neurons
AUTHOR(S): Yan, Chaohua; Fen, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy Of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**1998**), 33(7), 486-492
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The protective effects of d-3-n-butylphthalide (d-NBP) and l-3-n-butylphthalide (l-NBP) on hypoxia/hypoglycemia-induced cytotoxicity in primary cultured rat cortical neurons were studied. The results showed that d-NBP and l-NBP (1-100 μmol/L) inhibited hypoxia/hypoglycemia-induced lactate dehydrogenase (LDH) release, decreased the cell death rate and improved the damaged cellular morphol. at 10 μmol/L concentration The d-NBP, l-NBP and dl-NBP also significantly reduced the liberation of polyribosomes from the neuronal rough endoplasmic reticulum and the disaggregation of polyribosomes induced by hypoxia/hypoglycemia. These data suggested that d-NBP, l-NBP and dl-NBP could remarkably protect the cultured neurons against hypoglycemia-induced damage.

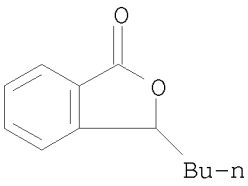
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, (±)-3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(protective effects of d-, l-, and dl-3-n-butylphthalide on neuronal damage induced by hypoxia/hypoglycemia in cultured rat cortical neurons)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

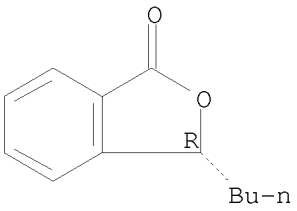


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



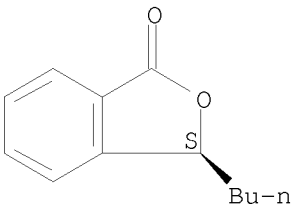
RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

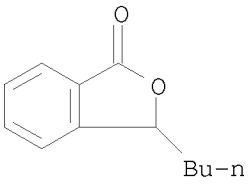


L9 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:147473 CAPLUS
DOCUMENT NUMBER: 124:305974
ORIGINAL REFERENCE NO.: 124:56371a,56374a
TITLE: Comparison of different 6-tert-butyldimethyl-silylated cyclodextrins as chiral stationary phases in GC
AUTHOR(S): Maas, Birgit; Dietrich, Armin; Mosandl, Armin
CORPORATE SOURCE: Inst. Lebensmittelchemie, J. W. Goethe-Universitaet, Frankfurt, D-60439, Germany
SOURCE: Journal of Microcolumn Separations (**1996**), 8(1), 47-56
CODEN: JMSEEJ; ISSN: 1040-7685
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Separation factors and thermodn. data for the separation of various chiral analytes
on different 6-TBDMS-derivatized γ(β)-cyclodextrin-phases were collected and discussed. Modifying the alkyl chain length of the substituents in position 2, and 3 of the cyclodextrin mol. or changing from β to γ-CD affects the separation properties extremely, whereas changing the chain length of acyl groups in position 2 and 3 hardly influences enantioselectivity.
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, 3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: ANT (Analyte); ANST (Analytical study)
(comparison of different 6-tert-butyldimethyl-silylated cyclodextrins as chiral stationary phases in gas chromatog. enantiomeric resolution of)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

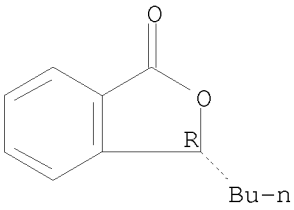


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)



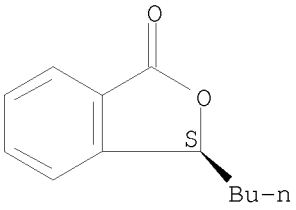
RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

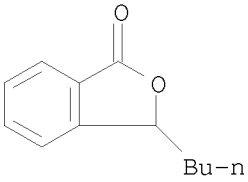


L9 ANSWER 23 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:451630 CAPLUS
DOCUMENT NUMBER: 123:131654
ORIGINAL REFERENCE NO.: 123:23071a,23074a
TITLE: Di-tert-butyldimethylsilylated cyclodextrins as chiral stationary phases: thermodynamic investigations
AUTHOR(S): Maas, Birgit; Dietrich, Armin; Beck, Thomas; Boerner, Susanne; Mosandl, Armin
CORPORATE SOURCE: Inst. Lebensmittelchemie, Biozentrum J. W. Goethe-Univ. Marie-Curie-Str. 9, Frankfurt/Main, D-60439, Germany
SOURCE: Journal of Microcolumn Separations (**1995**), 7(1), 65-73
CODEN: JMSEEJ; ISSN: 1040-7685
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Thermodn. data, which are derived from measurements of separation factors at different temps. for various chiral compds., show some expected, but also some surprising effects concerning the mechanism of chiral recognition for the cyclodextrin derivs. studied.
IT **3413-15-8**, (-)-3-Butylphthalide **6066-49-5**, (±)-3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: ANT (Analyte); ANST (Analytical study)
(thermodn. investigations for enantiosepns. using di-tert-butyldimethylsilylated cyclodextrins as chiral stationary phases)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

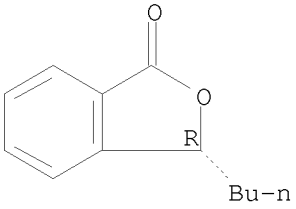


RN 6066-49-5 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl- (CA INDEX NAME)

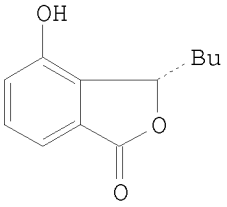


RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:76773 CAPLUS
DOCUMENT NUMBER: 112:76773
ORIGINAL REFERENCE NO.: 112:13115a,13118a
TITLE: Synthesis of (-)-3-butyl-4-hydroxyphthalide
AUTHOR(S): Ogawa, Yoshimitsu; Hosaka, Kunio; Chin, Masao; Mitsuhashi, Hiroshi
CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ami, 300-11, Japan
SOURCE: Heterocycles (**1989**), 29(5), 865-72
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:76773
GI



I

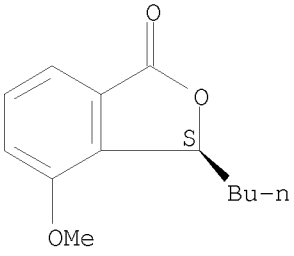
AB (-)-3-Butyl-4-hydroxyphthalide (I) was synthesized enantioselectively and its absolute stereochem. at C-3 was determined to be S.

IT **124831-75-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)

RN 124831-75-0 CAPLUS

CN 1(3H)-Isobenzofuranone, 3-butyl-4-methoxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

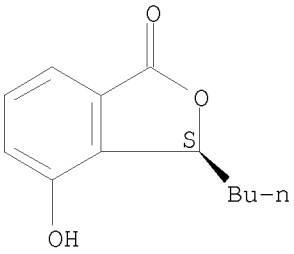


IT **74459-24-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and triflation of)

RN 74459-24-8 CAPLUS

CN 1(3H)-Isobenzofuranone, 3-butyl-4-hydroxy-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.

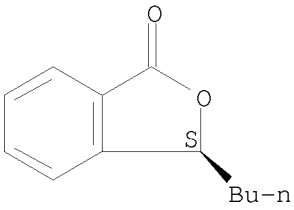


IT **3413-15-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 3413-15-8 CAPLUS

CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

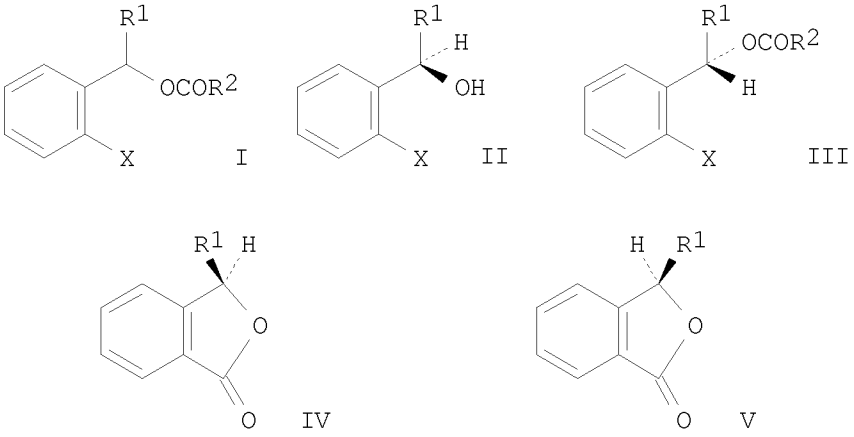
Absolute stereochemistry. Rotation (-).



ACCESSION NUMBER: 1997:480441 CAPLUS
DOCUMENT NUMBER: 127:94192
ORIGINAL REFERENCE NO.: 127:18116h,18117a
TITLE: Manufacture of optically active α-alkyl-2-halobenzyl alcohols and esters by enzymic hydrolysis and their use in manufacture of optically active 3-alkylphthalides
INVENTOR(S): Izumi, Taeko
PATENT ASSIGNEE(S): Kawaken Fine Chemicals Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09149791	A	19970610	JP 1995-312372	19951130 <--

PRIORITY APPLN. INFO.: JP 1995-312372 19951130
OTHER SOURCE(S): MARPAT 127:94192
GI



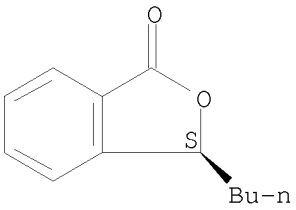
AB α-Alkyl-2-halobenzyl esters I (R1 = C1-4 alkyl; R2 = C1-18 alkyl, alkenyl, aryl; X = Br, I) are enzymically hydrolyzed to give (R)-α-alkyl-2-halobenzyl alcs. II (R1, X = same as above) and (S)-α-alkyl-2-halobenzyl esters III (R1, R2, X = same as above). II are cyclized by treating with CO in the presence of Pd compds. and tertiary phosphines to give (R)-3-alkylphthalides IV (R1 = same as above). III are hydrolyzed with alkalies or acids and the resulting (S)-α-alkyl-2-halobenzyl alcs. are cyclized by treating with CO in the presence of Pd. compds. and tertiary phosphines to give (S)-3-alkylphthalides V (R1 = same as above). 1-(2-Iodophenyl)ethyl butyrate was treated with pig liver esterase at 23° and pH 7.2 for 5 h to give 49% (S)-1-(2-iodophenyl)ethyl butyrate with 83% e.e. and 48% (R)-1-(2-iodophenyl)ethyl alc. (VI) with 49% e.e. Then, VI was treated with CO in the presence of Pd acetate, Ph3P, and Bu3N to give 78% (R)-3-methylphthalide with 86% e.e.

IT **3413-15-8P**, (S)-3-Butylphthalide **125412-70-6P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(manufacture of optically active α-alkyl-2-halobenzyl alcs. and esters by enzymic hydrolysis and their use in manufacture of optically active 3-alkylphthalides)

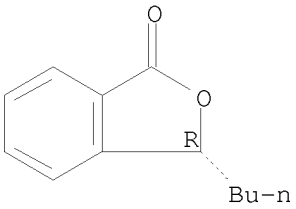
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

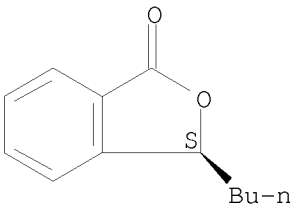
Absolute stereochemistry. Rotation (+).



L9 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:56566 CAPLUS
DOCUMENT NUMBER: 132:331477
TITLE: Modified cyclodextrins as versatile chiral stationary phases in flavor chemistry and life sciences
AUTHOR(S): Mosandl, A.; Podebrad, F.; Bartschat, D.; Kaunzinger, A.; Reichert, S.; Wust, M.
CORPORATE SOURCE: Institut fur Lebensmittelchemie, Biozentrum J.W. Goethe-Universitat, Frankfurt/Main, D-60439, Germany
SOURCE: Proceedings of the International Symposium on Cyclodextrins, 9th, Santiago de Comostela, Spain, May 31-June 3, 1998 (**1999**), Meeting Date 1998, 605-608. Editor(s): Labandeira, J. J. Torres; Vila-Jato, J. L. Kluwer Academic Publishers: Dordrecht, Neth.
CODEN: 68NHAE
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Modified cyclodextrins as chiral stationary phases in capillary gas chromatog. are proved to be powerful tools in the enantioselective anal. of different chiral volatiles, detecting origin specific enantiomeric distributions. In flavor chemical enantioselective anal. is used for authenticity assessment and biogenesis studies. In medicine, enantio-MDGC/MS serves to diagnostic and metabolic studies of inherited metabolic diseases.
IT **3413-15-8 125412-70-6**
RL: ANT (Analyte); ANST (Analytical study)
(modified cyclodextrins as versatile chiral stationary phases in flavor chemical and life sciences)

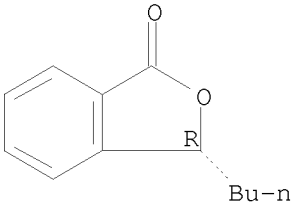
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

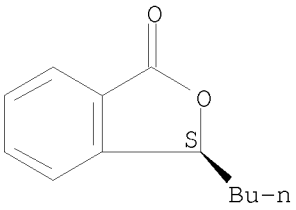
Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

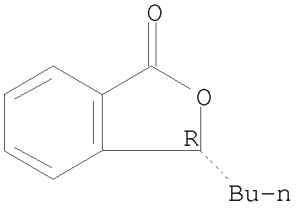
L9 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:402993 CAPLUS
DOCUMENT NUMBER: 131:213422
TITLE: Celery impact aroma compounds: structure, properties, analysis
AUTHOR(S): Bartschat, Dietmar; Wust, Matthias; Mosandl, Armin
CORPORATE SOURCE: Institut fur Lebensmittelchemie, Biozentrum, Johann Wolfgang Goethe-Universitat Frankfurt, Frankfurt/Main, 60439, Germany
SOURCE: Natural Product Analysis: Chromatography, Spectroscopy, Biological Testing, [Symposium], Wuerzburg, Germany, Sept. 1997 (**1998**), Meeting Date 1997, 49-50. Editor(s): Schreier, Peter. Vieweg: Wiesbaden, Germany.
CODEN: 67USA7
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Using enantioselective multidimensional gas chromatog. (enantio-MDGC) system, the genuine occurrence of 3-butylphthalide enantiomers and 3-butylhexahydrophthalide stereoisomers in celery-, celeriac-, celery seed- and fennel-exts. were determined Also, sensory characteristics and odor thresholds were evaluated via enantio-GC/olfactometry.
IT **3413-15-8P**, (S)-3-Butylphthalide **125412-70-6P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(celery impact aroma compds.)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

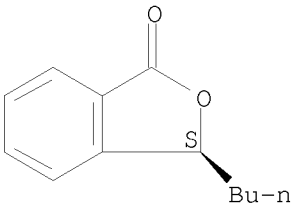


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:581929 CAPLUS
DOCUMENT NUMBER: 130:20473
TITLE: Effects of D-3-N-butylphthalide and L-3-N-butylphthalide on extracellular NO level and intracellular cGMP level in primary culture rat cortical neurons
AUTHOR(S): Yan, Chaohua; Feng, Yipu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**1998**), 33(6), 418-423
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The effects of d-3-N-butylphthalide (D-NBP) and l-3-N- butylphthalide (L-NBP) on extracellular NO level and intracellular cGMP level in primary culture rat cortical neurons were studied. The NO was measured by spectrophotometry and cGMP by RIA. When the primary culture of rat cerebral cortex neurons were exposed to hypoxia, hypoglycemia, NMDA, or KCl for 10 h, the D-NBP at 0.1-100 μmol/L significantly increased the extracellular NO and intracellular cGMP, while L-NBP showed an opposite effect. Since both compds. are neuroprotectants in these conditions, it appears that their activity is based on some other mechanism.
IT **3413-15-8**, (-)-3-Butylphthalide **125412-70-6**, (+)-3-Butylphthalide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of D- and L-3-butylphthalide on extracellular NO and intracellular cGMP levels in primary culture of rat cortical neurons)
RN 3413-15-8 CAPLUS

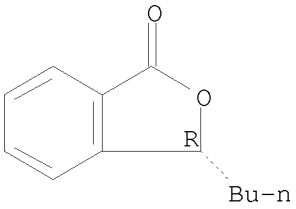
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



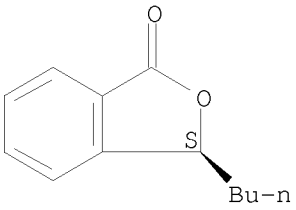
L9 ANSWER 29 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:762763 CAPLUS
DOCUMENT NUMBER: 128:97577
ORIGINAL REFERENCE NO.: 128:18945a,18948a
TITLE: Protective effects of d-3-n-butylphthalide and l-3-n-butylphthalide on neuronal damage induced by KCl and NMDA in cultured rat cortical neurons
AUTHOR(S): Yan, Chaohua; Zhang, Juntian; Feng, Yipu
CORPORATE SOURCE: Institute Materia Medica, Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (**1997**), 32(5), 340-346
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The protective effects of l-3-n-butylphthalide(l-NBP) and d-3-n-butylphthalide (d-NBP) on KCl (20 mmol L-1)- or NMDA (N-methyl-D-aspartate, 30 μmol L-1)-induced cytotoxicity in primary cultured rat cortical neurons were studied. Intracellular LDH release, percentage of cell death and cellular morphol. changes were used to evaluate the effect of drugs. l-NBP (1-100 μmol L-1) and d-NBP (1-100 μmol L-1) dose-dependently inhibited LDH release induced by NMDA (30 μmol L-1) in cultured rat cortical neurons with IC50 values of 4.89 μmol L-1 and 13.52 μmol L-1, resp., but not nimodipine (1-100 μmol L-1). The percent cell death was reduced with IC50 values of 44.37 and 49.78 μmol L-1, and the cellular morphol. was improved. The effects were similar to that of equal concentration of NAME (NG-nitro-L-arginine Me ester). l-NBP (10 μmol L-1), d-NBP (10 μmol L-1) and nimodipine (10 μmol L-1) also significantly inhibited intracellular LDH release and decreased in percent cell death induced by KCl (20 mmol L-1) in cultured neurons. The potencies of l-NBP and d-NBP were similar to that

of equal dose of nimodipine. The data suggest that 1-NBP and d-NBP can remarkably protect cultured neurons against the damage induced by KCl and NMDA.

IT **3413-15-8 125412-70-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(protective effects of d-3-n-butylphthalide and l-3-n-butylphthalide on neuronal damage induced by KCl and NMDA in cultured rat cortical neurons)

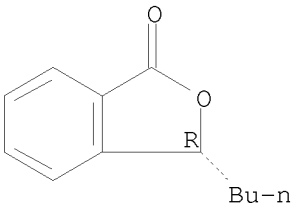
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:740710 CAPLUS
DOCUMENT NUMBER: 127:358234
ORIGINAL REFERENCE NO.: 127:70127a,70130a
TITLE: Stereoisomeric Flavor Compounds. 79. Simultaneous Enantio- selective Analysis of 3-Butylphthalide and 3-Butylhexahydro- phthalide Stereoisomers in Celery, Celeriac, and Fennel
AUTHOR(S): Bartschat, Dietmar; Beck, Thomas; Mosandl, Armin
CORPORATE SOURCE: Institut fuer Lebensmittelchemie Biozentrum, Johann Wolfgang Goethe-Universitaet Frankfurt, Frankfurt/Main, 60439, Germany
SOURCE: Journal of Agricultural and Food Chemistry (**1997**), 45(12), 4554-4557
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

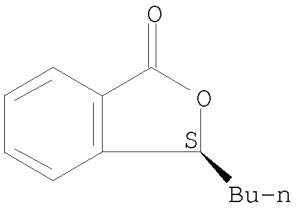
AB Using enantioselective multidimensional gas chromatog. with heptakis[2,3-di-O-acetyl-6-O-(tert-butyldimethylsilyl)]-β-cyclodextrin as the chiral stationary phase, the simultaneous anal. of the 3-butylphthalide enantiomers and all eight 3-butylhexahydrophthalide

stereoisomers was achieved. Enantiomeric distributions of compds. in celery, celeriac, celery seed, and fennel exts. were elucidated. Odor characteristics of compds. investigated are given.

IT **3413-15-8 125412-70-6**
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(simultaneous enantio- selective anal. of 3-butylphthalide and 3-butylhexahydro- phthalide stereoisomers in celery, celeriac, and fennel)

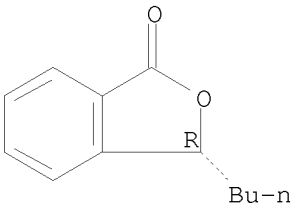
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:664629 CAPLUS
DOCUMENT NUMBER: 127:330602
ORIGINAL REFERENCE NO.: 127:64933a,64936a
TITLE: 3-Butyl(hexahydro)phthalides. Characteristic compounds of celery
AUTHOR(S): Bartschat, Dietmar; Mosandl, Armin
CORPORATE SOURCE: Institut Lebensmittelchemie, Johann Wolfgang Goethe-Universitat Frankfurt, Frankfurt/Main, D-60439, Germany
SOURCE: GIT Labor-Fachzeitschrift (**1997**), 41(9), 874-876
CODEN: GLFAF5
PUBLISHER: GIT Verlag
DOCUMENT TYPE: Journal
LANGUAGE: German

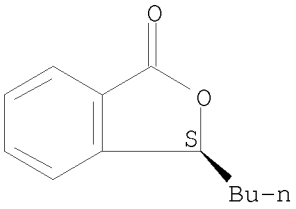
AB Enantioselective multidimensional GC (enantio-MDGC) was used for the simultaneous anal. of genuine 3-butyl(hexahydro)phthalides (I) and the sensual properties of natural stereoisomers were evaluated. Two enantiomers of 3-butylphthalide (II) and 8 stereoisomers of I were separated

by enantio-MDGC and the relative and absolute configuration of the compds. was determined by 1H-NMR. Enantio-MDGC was coupled with direct sensual detection for the evaluation of odor quality and odor thresholds. The stereoisomers 2' (3R,3aR,7aS) and 3 (3S,3aR,7aS) of I were not responsible for the odor of I in celery extract because their sensual relevance could be ignored (odor threshold > 125 ng). The odor-active stereoisomers 2 (3R,3aS,7aR), 4 (3S,3aR,7aR), 4' (3R,3aS,7aS), and 5 (3S,3aS,7aS) of I were not detected in celery extract The odor of 3S-II was more intensive than that of 3R-II and 3S-II was the predominant enantiomer of II in celery extract

IT **3413-15-8 125412-70-6**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(3-butyl(hexahydro)phthalides in celery)

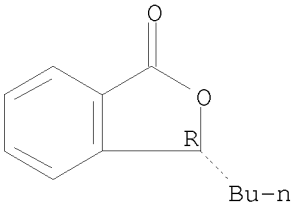
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:559620 CAPLUS
DOCUMENT NUMBER: 125:300725
ORIGINAL REFERENCE NO.: 125:56283a,56286a
TITLE: Chemoenzymic synthesis of optically active 3-methyl- and 3-butylphthalides
AUTHOR(S): Izumi, Taeko; Itou, Osamu; Kodera, Keiji
CORPORATE SOURCE: Dep. of Materials Sci. and Technology, Yamagata Univ., Yonezawa, 992, Japan
SOURCE: Journal of Chemical Technology & Biotechnology (**1996**), 67(1), 89-95
CODEN: JCTBED; ISSN: 0268-2575
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:300725

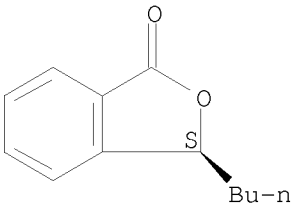
AB Optically active (S)-3-methylphthalide was synthesized by the enzymic reduction of 2-iodoacetophenone using baker's yeast, followed by palladium-catalyzed carbonylation under carbon monoxide. With enzymic

reduction using baker's yeast, however, 2-bromo- or 2-iodovalerophenones were not reduced, even after 25 days. On the other hand, the enantioselective hydrolysis of α-alkylated 2-halobenzyl acylates using pig liver esterase, horse liver esterase or lipase from Candida rugosa resulted in the formation of (R)-α-alkylated 2-halobenzyl alc. and (S)-acylate, and the following palladium-catalyzed carbonylation of the products yield the (R)- and (S)-3-alkylated phthalides, resp.

IT **3413-15-8P 125412-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(chemoenzymic synthesis of Me and butylphthalides)

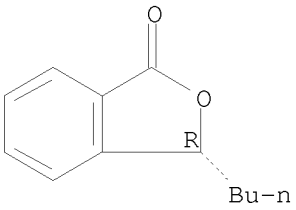
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:327861 CAPLUS
DOCUMENT NUMBER: 125:84901
ORIGINAL REFERENCE NO.: 125:16015a,16018a
TITLE: Stereoisomeric flavor compounds. LXXIII: 3-butylphthalide: chirospecific analysis, structure and properties of the enantiomers
AUTHOR(S): Bartschat, Dietmar; Maas, Birgit; Smietana, Sabine; Mosandl, Armin
CORPORATE SOURCE: Inst. fuer Lebensmittelchemie, Johann Wolfgang Goethe-Univ. Frankfurt, Frankfurt/Main, 60439, Germany
SOURCE: Phytochemical Analysis (**1996**), 7(3), 131-135
CODEN: PHANEL; ISSN: 0958-0344
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

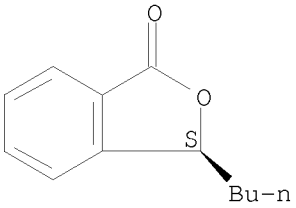
AB Using enantioselective gas chromatog. (GC) with an octakis-(2,6-di-O-tert-butyldimethylsilyl)-γ-cyclodextrin column, the direct enantioselective anal. of 3-butylphthalide enantiomers was achieved. Investigations relating to their sensory characteristics and odor thresholds were carried out via enantioselective gas chromatog./olfactometry. In order to elucidate stereochem. features, the

lactone structure of racemic 3-butylphthalide was hydrolyzed and the carboxy function protected as an isopropylester; the hydroxy function at C-3 was esterified with (R)-2-phenylpropionic acid. The resulting diastereomeric esters were separated and isolated by high performance liquid chromatog. Absolute configurations were derived from 1H-NMR studies according to the Helmchen model, subsequently followed by ester cleavage and recyclization to the corresponding 3-butylphthalide enantiomers. Investigation of the essential oil of celery seed show enantiomeric distributions in the range of 95:5 in favor of the (3S)-enantiomer. This enantiomer shows a significant lower GC odor threshold value than does the (3R)-enantiomer.

IT **3413-15-8P 125412-70-6P**
RL: ANT (Analyte); BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective gas chromatog. of butylphthalides)

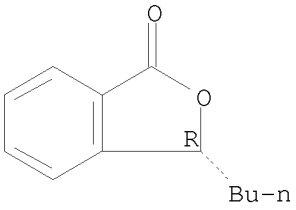
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

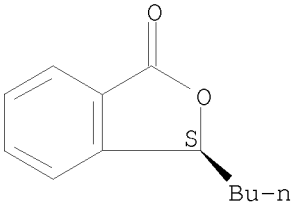
Absolute stereochemistry. Rotation (+).



L9 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:198474 CAPLUS
DOCUMENT NUMBER: 124:343016
ORIGINAL REFERENCE NO.: 124:63707a,63710a
TITLE: Efficient general asymmetric syntheses of 3-substituted 1(3H)-isobenzofuranones in very high enantiomeric excess
AUTHOR(S): Ramachandran, P. Veeraraghavan; Chen, Guang-Ming; Brown, Herbert C.
CORPORATE SOURCE: H.C. Brown and R. B. Wetherill Lab. Chem., Purdue Univ., West Lafayette, IN, 47907-1393, USA
SOURCE: Tetrahedron Letters (**1996**), 37(13), 2205-8
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier

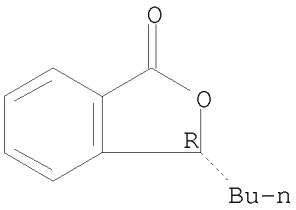
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:343016
AB The intermol. asym. reduction of Me o-(1-oxoalkyl)benzoates with β-chlorodiisopinocampheylborane provides, after workup, 3-alkylphthalides in ≥97% ee. Unfortunately, this procedure is not as efficient for the preparation of 3-arylphthalides. However, an intramol. reduction of B-(o-benzoylbenzoyloxy)diisopinocampheylborane, readily prepared by the treatment of o-benzyl benzoic acid with diisopinocampheylborane, provides 3-phenylphthalide in ≥96% ee.
IT **3413-15-8P 125412-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

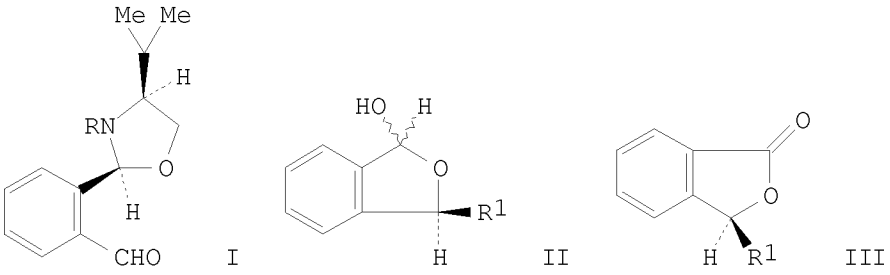


RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:194072 CAPLUS
DOCUMENT NUMBER: 116:194072
ORIGINAL REFERENCE NO.: 116:32877a,32880a
TITLE: Highly diastereoselective reaction of chiral o-[2-(1,3-oxazolidinyl)]benzaldehydes with alkylmetallic reagents: synthesis of chiral 3-substituted phthalides
AUTHOR(S): Takahashi, Hiroshi; Tsubuki, Takeshi; Higashiyama, Kimio
CORPORATE SOURCE: Fac. Pharm. Sci., Hoshi Univ., Tokyo, 142, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (**1991**), 39(12), 3136-9
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:194072
GI

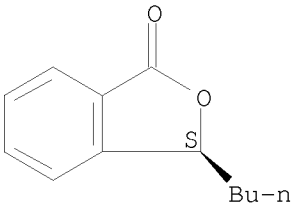


AB o-[2-(1,3-Oxazolidinyl)]benzaldehydes I (R = Me, Et, CHMe2) react with alkylmetallic reagents (Bu2CuLi, Et2Zn, MeMgBr, BuMgCl) and p-toluenesulfonic acid to give hydroxyoxaindans II (R1 = Me, Et, Bu) which were oxidized to give chiral phthalides III.

IT **3413-15-8P 125412-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

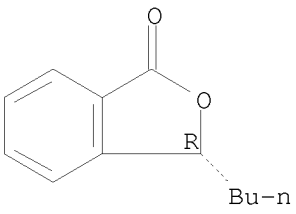
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



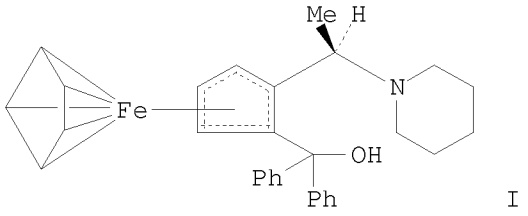
RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

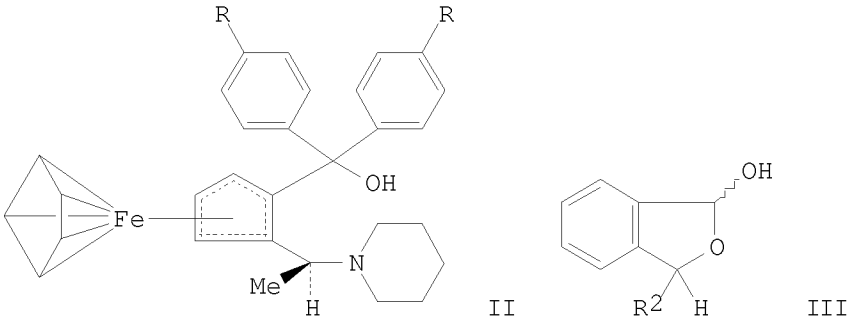


L9 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:41215 CAPLUS
DOCUMENT NUMBER: 116:41215
ORIGINAL REFERENCE NO.: 116:7064h,7065a
TITLE: A facile synthesis of optically active 3-ethyl- and 3-butylphthalides via catalytic enantioselective addition of dialkylzinc reagents to o-phthalaldehyde
AUTHOR(S): Watanabe, Makoto; Hashimoto, Norifumi; Araki, Shuki; Butsugan, Yasuo
CORPORATE SOURCE: Dep. Appl. Chem., Nagoya Inst. Technol., Nagoya, 466,

Japan
SOURCE: Journal of Organic Chemistry (**1992**), 57(2), 742-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:41215
GI



I



II

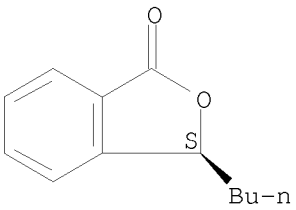
III

AB Chiral 1,2-disubstituted ferrocenyl amino alcs. I and II (R = H, OMe, Cl) catalyzed highly enantioselective addition of dialkylzinc reagents to phthalaldehyde to afford optically active lactols III (R1 = Et, Bu) with >88% enantiomeric excess (ee). In particular, the catalyst II (R = Cl) afforded III (R1 = Et) in 98% ee and 3-n-butyllactol III (R1 = Bu) in 94% ee. Oxidation of the lactols with Ag2O afforded highly optically pure phthalides.

IT **3413-15-8P 125412-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

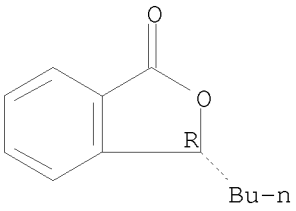
RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

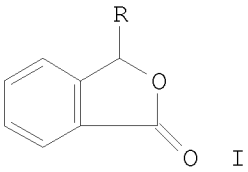


RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:471293 CAPLUS
DOCUMENT NUMBER: 115:71293
ORIGINAL REFERENCE NO.: 115:12315a,12318a
TITLE: Catalytic enantioselective synthesis of optically active phthalides
AUTHOR(S): Soai, Kenso; Hori, Hiroshi; Kawahara, Masato
CORPORATE SOURCE: Fac. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan
SOURCE: Tetrahedron: Asymmetry (**1991**), 2(4), 253-4
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:71293
GI

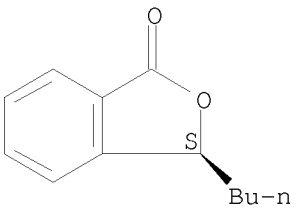


AB Optically active phthalides (R)-(+)-I (R = Et, Bu) were prepared in three steps. The key step was the alkylation of 2-bromobenzaldehyde with R2Zn in the presence of (1R,2S)-N,N-dibutylnorephedrine (DBNE) to give 2-BrC6H4CHR(OH) (II) with high enantioselectivity. II was subsequently formylated with DMF and then oxidized to I. (S)-(-)-I (R = Bu) was obtained using (1S,2R)-DBNE and Bu2Zn.

IT **3413-15-8P 125412-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 3413-15-8 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 125412-70-6 CAPLUS
CN 1(3H)-Isobenzofuranone, 3-butyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).